# 6-heptyltetrahydro-2H-thiopyran-2-one

**Inchi:** InChI=1S/C12H22OS/c1-2-3-4-5-6-8-11-9-7-10-12(13)14-11/h11H,2-10H2,1H3
**InchiKey:** SYVWURCNFWCYOL-UHFFFAOYSA-N
**Formula:** C12H22OS
**SMILES:** CCCCCCCC1CCCC(=O)S1
**Mol. weight [g/mol]:** 214.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -8.12 | kJ/mol | Joback Method |
| hf | -329.13 | kJ/mol | Joback Method |
| hfus | 21.84 | kJ/mol | Joback Method |
| hvap | 52.79 | kJ/mol | Joback Method |
| log10ws | -4.51 | | Crippen Method |
| logp | 4.159 | | Crippen Method |
| mcvol | 187.000 | ml/mol | McGowan Method |
| pc | 2191.78 | kPa | Joback Method |
| rinpol | 1789.00 | | NIST Webbook |
| ripol | 2473.00 | | NIST Webbook |
| ripol | 2473.00 | | NIST Webbook |
| tb | 609.16 | K | Joback Method |
| tc | 826.54 | K | Joback Method |
| tf | 384.05 | K | Joback Method |
| vc | 0.694 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 490.53 | J/mol×K | 609.16 | Joback Method |
| cpg | 510.37 | J/mol×K | 645.39 | Joback Method |
| cpg | 529.13 | J/mol×K | 681.62 | Joback Method |
| cpg | 546.81 | J/mol×K | 717.85 | Joback Method |
| cpg | 563.43 | J/mol×K | 754.08 | Joback Method |
| cpg | 579.00 | J/mol×K | 790.31 | Joback Method |
| cpg | 593.52 | J/mol×K | 826.54 | Joback Method |

# Sources

| | |
|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R301458&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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